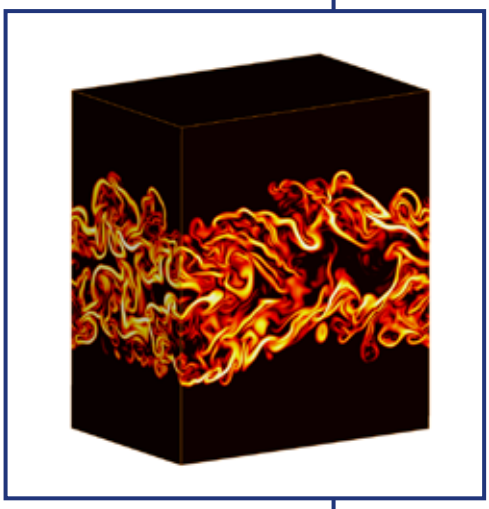
Combustion Simulation: Turbulent Non-premixed Flames

Advancing basic understanding of turbulent combustion and developing predictive combustion models are essential to deliver reliable data for manufacturer design of combustors and to limit hardware testing costs.



Scalar dissipation rate field (indication of local mixing intensity) in a turbulent plane jet flame.

The Challenge

Combustion equipment that uses fuel efficiently and minimizes harmful emissions is essential to building a secure, sustainable energy infrastructure. Faced with stiff global competition and concern over harmful emissions, makers of combustion devices (e.g., internal combustion engines, power turbines, industrial furnaces) are challenged to improve the reliability, fuel efficiency, and emissions performance of their products. High-performance computing is an unmatched tool for advancing combustion science via predictive models that will revolutionize combustion equipment design and performance.

Understanding the mechanisms governing flame extinction and re-ignition in a turbulent environment is key to developing those models. In many common combustors, fuel and air are injected separately into the combustion chamber rather than being premixed. Therefore, fundamental questions about the combustion process revolve around the rate at which the fuel and air mix in the chamber. Rapid mixing produces rapid energy release, allowing the use of smaller combustion chambers and reducing emissions. However, above a critical level, rapid mixing and the associated turbulence can extinguish combustion in areas of the flame or even destabilize the entire flame. Extinguished fuel–air pockets that fail to re-ignite quickly are exhausted from the combustor, and abundant extinguished pockets that do not re-ignite can halt combustion altogether. Thus extinction adversely affects energy efficiency, emissions, and safety.

Research at the NLCF

Researchers are using the NLCF massively parallel supercomputers to perform the first 3-dimensional turbulent direct numerical simulation (DNS) of a non-premixed H2/CO/N2–air flame with detailed chemistry to study extinction and reignition mechanisms. The DNS is part of a parametric study performed on three different Office of Science computing platforms: the IBM SP at NERSC (FY 2005 INCITE award), the HP Itanium-2 cluster at PNNL, and the ORNL CrayX1E and XT3.

The simulation is performed using the Sandia DNS code S3D, which has been used extensively to investigate fundamental turbulence-chemistry interactions. The chosen physical configuration corresponds to a temporally-evolving plane jet flame (See the figure).
This DNS clarifies extinction and reignition mechanisms in a turbulent environment by including detailed chemistry (i.e., capable of fully representing burning and igniting chemical states), heat release, and realis-

tic thermochemical properties. Unlike previous DNS studies, this one permits reignition to occur by either autoignition or flame propagation. Statistics will be obtained for the occurrence of the different modes of reignition as a function of key flow and flame parameters.

The resulting numerical benchmark data will complement a library of experimental flame data on non-premixed turbulent combustion. They will be shared with an international collaboration of researchers working to advance the predictive capability of combustion models. A key limitation in existing models is their inability to describe combustion phenomena involving coupling of finite-rate chemistry with turbulence. It is exactly this type of information that the DNS will provide.

How NCCS Enables this Research

These simulations require millions of cpu-hours with between 50 and 500 million grid points on terascale computers. On the NLCF computers, it is possible to run the process in weeks rather than in months or years. To achieve the needed fidelity in a reasonable amount of processing time, it is advantageous to perform these simulations on a vector processing architecture (one that operates on a large array of values simultaneously, rather than on just a few values). Test runs have shown the DNS code S3D runs four times faster on the vector system than on a non-vector system. The Cray X1E is the largest vector system in the United States that is available for open research.

A production calculation using 100 million grid points has been performed on the NLCF's computing resources. The preliminary calculations indicate that both diffusivity and the strong interplay between reaction and diffusion in non-premixed flames affect mixing time scales. The findings underline the importance of considering the interplay of diffusion and reaction, particularly where strong finite-rate chemistry effects are involved. At present, highly resolved simulations of this sort are the only way to obtain this type of information.

Impact of Combustion Simulations

Advances in combustion device design have traditionally been incremental—making small changes from previous designs and then building hardware to test the results. This slow, costly approach is ill-suited to the challenges of modern manufacturing and global competition. Reliable, detailed computer modeling will enable designers to explore radical design changes and complex control strategies rapidly with limited need for hardware testing.

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